TITLE: **ADVANCED COMPUTATIONAL MODEL FOR THREE-PHASE SLURRY REACTORS**

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ABSTRACT

OBJECTIVES

The general objective of this project is to provide the needed fundamental understanding of three-phase slurry reactors in Fischer-Tropsch (F-T) liquid fuel synthesis. The other main goal is to develop a computational capability for predicting the transport and processing of three-phase coal slurries. The specific objectives are:

- To develop a thermodynamically consistent rate-dependent anisotropic model for multiphase slurry flows with and without chemical reaction for application to coal liquefaction. Also to establish the material parameters of the model.
- To provide experimental data for phasic fluctuation and mean velocities, as well as the solid volume fraction in the shear flow devices.
- To develop an accurate computational capability incorporating the new rate-dependent and anisotropic model for analyzing reacting and nonreacting slurry flows, and to solve a number of technologically important problems related to Fischer-Tropsch (F-T) liquid fuel production processes.
- To verify the validity of the developed model by comparing the predicted results with the performed and the available experimental data under idealized conditions.

ACCOMPLISHMENTS TO DATE

An Eulerian-Largrangian formulation for analyzing three-phase slurry flows in a bubble column is developed. The approach uses an Eulerian analysis of liquid flows in the bubble column, and makes use of the Lagrangian trajectory analysis for the motions of bubbles and particles. The developed method accounts for the two-way interactions of the three-phase flows.

A computational model for two-phase flow was developed and the flows in horizontal and

inclined ducts were analyzed. The results were compared with the available experimental data and earlier model predictions and good agreements were observed. A computational model for analyzing two-phase solid-liquid flows at various mass loading ratios was also developed and was successfully used to predict flow parameters down an inclined chute.

An experimental set-up for generating a two-dimensional bubble column for detail studies is fabricated. The diagnostic methods for quantitative measurements are developed.

Progress was also made in studying two-phase bubbly flows using the volume-of-fluid (VOF) approach. The Largragian trajectory of a dilute concentration of the solid phase is also studied. In a related modeling effort, progress was made in developing a rate dependent thermodynamically consistent model for slurry flows. The new model includes the effect of phasic interactions and appears to lead to anisotropic effective stress tensor. The formulation is being extended to cover three-phase liquid-gas-solid flows.

Progress was also made in analyzing turbulent two-phase flows with heat transfer. We developed an Eulerian/Lagrangian approach including the two-way interaction for two-phase flows. The model considers the thermal turbulent field characteristics and includes an explicit equation for temperature fluctuation in addition to the turbulence kinetic energy and time scales of the flow and thermal field fluctuations.

Progress was also made in measuring concentration and velocity profiles of particles of different sizes near a solid wall in a duct flow. The result shows that small particles have diffusion dominated concentration profiles near the wall, while the larger particles could acquire an inertial dominated counter gradient profile.

SIGNIFICANCE TO FOSSIL ENERGY PROGRAM

Converting coal to liquid hydrocarbon fuel by direct and indirect liquefaction processes has been of great concern to the development of coal-based energy systems. While the direct hydrogenation has been quite successful and was further developed in various forms, use of slurry phase Fischer-Tropsch (F-T) processing is considered a potentially more economical scheme to convert synthesis gas into liquid fuels. Slurry transport and processing and pneumatic transport of particles play a critical role in the operation, efficiency, safety and maintenance of these advanced coal liquefaction and coal-based liquid fuel production systems. Therefore, a fundamental understanding of reacting coal slurries will have a significant impact on the future of environmentally acceptable liquid fuel generation from coal.

Particle-particle and particle-gas/liquid interactions strongly affect the performance of three-phase slurry reactors used in coal conversion processes and are crucial to the further development of coal-based synthetic hydrocarbon fuel production systems. The scientific knowledge base for these processes, however, is in its infancy. Therefore, most current techniques were developed on an *ad hoc* and trial and error basis. This project is concerned with for providing the needed fundamental understanding of the dynamics of chemically active slurries and three-phase mixtures. In particular, a computational model for predicting the behavior of dense mixtures in coal liquefaction, gasification and liquid fuel production equipment will be developed.

PLANS FOR THE COMING YEAR

- To finalize and publish the thermodynamical consistent and anisotropic model for multiphase

slurry flows.

- To finalize the volume of the fluid model for bubbly flows and to simulate technologically important problems related to Fischer-Tropsch (F-T) liquid fuel production processes.
- To perform experimental measurements of the phasic properties in the simple shear flow device and in the plane bubble column.

ARTICLES, PRESENTATIONS AND STUDENT SUPPORT

Journals Articles (peer reviewed)

He, C. and Ahmadi, G., Particle Deposition in a Nearly Developed Turbulent Duct Flow with Electrophoresis, J. Aerosol Science, Vol. 30, pp. 739-758 (1999).

Cao, J. and Ahmadi, G., Gas-Particle Two-Phase Flow in Horizontal and Inclined Ducts, Int. J. Engng. Sci, Vol. 38, pp. 1961-1981 (2000).

Zhang, H. and Ahmadi, G., Aerosol Particle Transport and Deposition in Vertical and Horizontal Turbulent Channel Duct Flows, J. Fluid Mechanics, Vol. 406, pp. 55-88 (2000).

Fan, F-G. and Ahmadi, G., Wall Deposition of Small Ellipsoids from Turbulent Air Flows-A Brownian Dynamics Simulation, J. Aerosol Sci., Vol. 31, pp. 1205-1229 (2000).

Soltani, M. and Ahmadi, G., Direct Numerical Simulation of Curly Fibers in Turbulent Channel Flow, Aerosol Science Technology, Vol. 33, pp. 392-418 (2000).

Ahmadi, G., He, C., Ban, H. and Stencel, J.M., Air Flow and Particle Transport in Triboelectric Coal/Ash Cleaning System-Counter Flowing Straight Duct Design, Particulate Science Technology, Vol. 18, pp. 213-256 (2000).

Shams, M., Ahmadi, G. and Rahimzadeh, H., A Sublayer Model for Deposition of Nano- and Micro-Particles in Turbulent Flows, Chemical Engineering Science, Vol. 55, pp. 6097-6107 (2000).

Zhang, H., Ahmadi, G. Fan, F.-G. and McLaughlin, J.B., Ellipsoidal Particles Transport and Deposition in Turbulent Channel Flows, International Journal Multiphase Flows, Vol. 27, pp. 971-1009 (2001).

Zhang, H. and Ahmadi, G., Particles Transport and Deposition in the Hot-Gas Filter Vessel at Wilsonville, Powder Technology, Vol. 116, pp. 53-68 (2001).

Shams, M., Ahmadi, G. and Rahimzadeh, H., Transport and Deposition of Flexible fibers in Turbulent Duct Flows, Journal of Aerosol Science, Vol. 32, pp. 525-547 (2001).

Ahmadi, G. and C. He, Simulation of Particles Transport and Deposition in a Combustor, Chemical

Engineering Communication, Vol. 187, pp. 23-53 (2001).

Mansoori, Z., Saffar-Avval, M., Basirat Tabrizi, H and Ahmadi, G., Modeling of Heat Transfer in Turbulent Gas-Solid Flow, International Journal Heat Mass and Transfer, Vol. 45, pp. 1173-1184 (2002).

Conference Presentations

G. Ahmadi and J. Cao, "Anisotropic Model for Granular and Dense two-Phase Flows," 1999 ASME Mechanics and Materials Conference, Blacksburg, VA, June 27-30, 1999.

G. Ahmadi, K. Elliott and W. Kvasnak, "An Experimental Study of Granular Flow in a Couette Flow Device," 1999 ASME Mechanics and Materials Conference, Blacksburg, VA, June 27-30, 1999.

C. He and G. Ahmadi, "Modeling of Particle Dispersion and Deposition with Thermophoresis in a Controlled Profile Combustor," 18th Annual Conference of the American Association for Aerosol Research, AAAR '99, Tacoma. WA, October 11-15, 1999.

H. Zhang and G. Ahmadi, "Aerosol Particle Removal and Re-entrainment in Turbulent Channel Flows," 18th Annual Conference of the American Association for Aerosol Research, AAAR '99, Tacoma. WA, October 11-15, 1999.

H. Zhang and G. Ahmadi, F. Fan and J.B. McLaughlin, "Analysis of the Motion of Ellipsoidal Particle in Turbulent Channel Flows," 52st Annual Meeting of American Physical Society, Division of Fluid Dynamics, New Orleans, LA, November 21-23, 1999.

P.V. Skudarnov, L.L. Regel, W. R. Wilcox and G. Ahmadi, "Numerical Modeling and Flow Visualization in the Gradient Freeze Configuration During Centrifugation," Fourth International Workshop on Materials Processing at High Gravity, Clarkson University, Potsdam, NY, May 29-June 2, 2000.

A.R. Mazaheri, H. Zhang and G. Ahmadi, "A Centrifual Filtration Concept for Hot-Gas Cleaning," Fourth International Workshop on Materials Processing at High Gravity, Clarkson University, Potsdam, NY, May 29-June 2, 2000.

G. Ahmadi, "Advanced Computational Model for Three-Phase Slurry Reactors," Abstract and Research Accomplishments of University Coal Research Projects, pp. 91-91, University Coal Research Contractors Review Conference, NETL, Pittsburgh, PA, June 6-7, 2000.

G. Ahmadi and H. Zhang, "Resuspension of Particles in Turbulent Flows," Seventh International Symposium on Particles on Surfaces: Detection, Adhesion and Removal, Newark, NJ, June 19-21, 2000.

G. Ahmadi and H. Zhang, "Hot-Gas Flow and Particle Transport and Deposition in the Filter Vessel at Wilsonville," Seventeenth Annual International Pittsburgh Coal Conference, Pittsburgh, PA,

September 11-14, 2000.

A.R. Mazaheri and G. Ahmadi, "Computational Modeling of a Centrifual Filtration System," 19th Annual Conference of the American Association for Aerosol Research, AAAR 2000, St. Louis, MO, November 6-10, 2000.

D.J. Schmidt, G. Ahmadi, and G. Schmidt, "Dispersion of Droplets in a Turbulent Spray," 19th Annual Conference of the American Association for Aerosol Research, AAAR 2000, St. Louis, MO, November 6-10, 2000.

M. Shams, G. Ahmadi and H. Rahimzadeh, "Transport and Deposition of Flexible Fibers in Turbulent Flows," 19th Annual Conference of the American Association for Aerosol Research, AAAR 2000, St. Louis, MO, November 6-10, 2000.

H. Zhang, G. Ahmadi, R. Han and B.J. Greenspan, "Impact Breakup of Particle Pairs," 19th Annual Conference of the American Association for Aerosol Research, AAAR 2000, St. Louis, MO, November 6-10, 2000.

H. Zhang, G. Ahmadi, R. Han and B.J. Greenspan, "Breakup of Pairs of Attached Particles in Simple Shear Flows," 19th Annual Conference of the American Association for Aerosol Research, AAAR 2000, St. Louis, MO, November 6-10, 2000.

M. Shams, G. Ahmadi and C. Liu, "Nano- and Micro-Particle Transport and Deposition in Turbulent Flows," Annual Technical Meeting of the Center for Advanced Material Processing (CAMP), Saratoga Spring, NY, May 14-16, 2001.

X. Zhang and G. Ahmadi, "Gas-Liquid-Particle three-Phase Turbulent Flow in a Bubble Column," Annual Technical Meeting of the Center for Advanced Material Processing (CAMP), Saratoga Spring, NY, May 14-16, 2001.

D.J. Schmidt, G. Ahmadi, and G. Schmidt, "Lagrangian PDF: Application to Multiphase Spray Simulation," 4th International Conference on Multiphase Flows, ICMF' 2001, New Orleans, LA, May 27-June 1, 2001.

C. Liu and G. Ahmadi, "Transport and Deposition of Atmospheric Particles Near a Building Model," 4th International Conference on Multiphase Flows, ICMF' 2001, New Orleans, LA, May 27-June 1, 2001.

M. Shams, G. Ahmadi and H. Rahimzadeh, "Flexible Fiber Motion in Turbulent Flows," 4th International Conference on Multiphase Flows, ICMF' 2001, New Orleans, LA, May 27-June 1, 2001.

G. Ahmadi, "Advanced Computational Model for Three-Phase Slurry Reactors," University Coal Research/HBCU Contractors Review Conference, NETL, Pittsburgh, PA, June 5-6, 2001.

A. Sadiki and G. Ahmadi, "A Thermodynamical Formulation for Chemically Active Multiphase Flows," Trends in Numerical and Physical Modeling for Industrial Multiphase Flows, Institut d'Etudes Scientifiques de Cargese (Corse), France. September 26-28, 2001.

A.R. Mazaheri and G. Ahmadi, "Computational Modeling of Gas Flow in an Industrial Filter Vessel," 20th Annual Conference of the American Association for Aerosol Research, AAAR 2001, Portland, Oregon, October 15-19, 2001.

A.R. Mazaheri and G. Ahmadi, "Particle Transport, Deposition and Removal with Bounce in Turbulent Channel Flow," 20th Annual Conference of the American Association for Aerosol Research, AAAR 2001, Portland, Oregon, October 15-19, 2001.

X. Zhang and G. Ahmadi, "Gas-Particle Two-Phase Flow in a Horizontal Channel," 20th Annual Conference of the American Association for Aerosol Research, AAAR 2001, Portland, Oregon, October 15-19, 2001.

C. He, and G. Ahmadi, "Particle Dispersion and Deposition in a Sudden Expansion Turbulent Pipe Flow with Electrophoresis,"20th Annual Conference of the American Association for Aerosol Research, AAAR 2001, Portland, Oregon, October 15-19, 2001.

D.J. Schmidt, G. Ahmadi, and G. Schmidt, "Dispersion and Breakup of Deformable Droplets in a Turbulent Spray," 20th Annual Conference of the American Association for Aerosol Research, AAAR 2001, Portland, Oregon, October 15-19, 2001.

G. Ahmadi, "Three-Phase Slurry Reactors," Center for Advanced Materials Processng (CAMP), Annual Fall Meeting, Clarkson University, Potsdam, New York, October 17-19, 2001.

G. Ahmadi, "Computational Modeling of Particle Transport and Deposition," Symposium on Indoor and Urban Environmental Systems, Syracuse University, Syracuse, New York, October 30-31, 2001.

G. Ahmadi and H. Zhang, "Particle Entrainment in Turbulent Flows," 25th Annual Meeting of Adhesion Society and the Second Word Congress on Adhesion and Related Phenomena (WCARP-II), Orlando, FL, February 10-14, 2002.

G. Ahmadi and Shiguang Guo, "Adhesion and Detachment of Bumpy Particle In Turbulent Flows - Effects of Electrostatic and Capillary Forces," 25th Annual Meeting of Adhesion Society and the Second Word Congress on Adhesion and Related Phenomena (WCARP-II), Orlando, FL, February 10-14, 2002.

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